

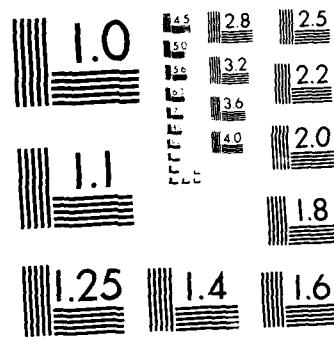
HD-H193 684 MOLECULAR INTERACTIONS WITH MANY-BODY METHODS(U) 171
FLORIDA UNIV GAINESVILLE R J BARTLETT 04 MAR 88
AFOSR-TR-88-0679 AFOSR-85-0011

UNCLASSIFIED

F/G 7/4

NL





UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

(2)

REPORT DOCUMENTATION PAGE

AD-A195 684

1b. RESTRICTIVE MARKINGS

3. DISTRIBUTION/AVAILABILITY OF REPORT
Approved for public release,
distribution is unlimited.

2d. DECLASSIFICATION / DOWNGRADING SCHEDULE

4. PERFORMING ORGANIZATION REPORT NUMBER(S)

5. MONITORING ORGANIZATION REPORT NUMBER(S)

AFOSR-TR- 88-0679

6a. NAME OF PERFORMING ORGANIZATION
Univ of Florida6b. OFFICE SYMBOL
(If applicable)7a. NAME OF MONITORING ORGANIZATION
AFOSR/NP6c. ADDRESS (City, State, and ZIP Code)
219 Grinter Hall
Gainesville, FL 326117b. ADDRESS (City, State, and ZIP Code)
Building 410, Bolling AFB DC
20332-64488a. NAME OF FUNDING / SPONSORING
ORGANIZATION
AFOSR8b. OFFICE SYMBOL
(If applicable)
NP9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
AFOSR-85-0011

8c. ADDRESS (City, State, and ZIP Code)

Building 410, Bolling AFB DC
20332-6448

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO. 61102F PROJECT NO. 2301 TASK NO. A4 WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)

(U) MOLECULAR INTERACTIONS WITH MANY-BODY METHODS

12. PERSONAL AUTHOR(S)

Dr Rodney J. Bartlett

13a. TYPE OF REPORT
FINAL

13b. TIME COVERED

FROM 1 Nov 84 TO 31 Oct 87

14. DATE OF REPORT (Year, Month, Day)

4 Mar 88

15. PAGE COUNT

4

16. SUPPLEMENTARY NOTATION

17. COSATI CODES

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)

| FIELD | GROUP | SUB-GROUP |
|-------|-------|-----------|
| 20 | 08 | |
| | | |

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This report summarized publications and invited presentations supported by our AFOSR grant on "Molecular Interactions with Many-Body Methods." In this effort new many-body methods have been developed to treat open-shell molecules; to apply to properties like moments, polarizabilities, hyperpolarizabilities, spin-densities and spin-spin coupling constants; infra-red spectra; and a variety of applications to interesting molecules including the unknown metastable N₂H₃ system. The latter molecule, though isoelectronic with ozone and cyclopropane is not known experimentally. However, we find that it should exist in three stable structures. Furthermore, we have predicted its IR spectra to aid in its experimental identification, which should be possible in matrix isolation. Other applications work has focused on the accurate, numerical orbital treatment of anions. (M.J.M.)

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT

 UNCLASSIFIED/UNLIMITED SAME AS RPT DTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION

UNCLASSIFIED

22a. NAME OF RESPONSIBLE INDIVIDUAL

R E KELLEY

22b. TELEPHONE (Include Area Code)

(202) 767-4908

22c. OFFICE SYMBOL

AFOSR/NP

I. PUBLICATIONS AND PRESENTATIONS SUPPORTED BY AFOSR (1986-present)

L. Adamowicz and R.J. Bartlett, "Very Accurate Coupled Cluster Calculations for Diatomic Systems with Numerical Orbitals," Nobel Laureate Symposium on Applied Quantum Chemistry, ed. V.H. Smith, H.F. Schaefer III, and K. Morokumo, Reidel, Dordrecht, The Netherlands, pg. 111 (1986).

S. Kucharski and R.J. Bartlett, "Fifth-Order Many-Body Perturbation and Its Relationship to Various Coupled Cluster Approaches," in Advances in Quantum Chemistry, 18, 281 (1986).

G.W. Trucks and R.J. Bartlett, "Isomers of Si_2C_2 : An MBPT Study," Mulliken Issue, J. Mol. Structure (Theochem) 135, 423 (1986).

H. Sekino and R.J. Bartlett, "Hyperpolarizabilities of the Hydrogen Fluoride Molecule: A Discrepancy Between Theory and Experiment?" J. Chem. Phys. 84, 2726 (1986).

D.H. Magers, R.J. Harrison and R.J. Bartlett, "Isomers and Excitation Energies of C_4 ," J. Chem. Phys. 84, 3284 (1986).

L. Adamowicz and R.J. Bartlett, "Numerical Coupled Hartree-Fock Study of the Total Electronic and Nuclear Parallel Polarizability and Hyperpolarizabilities for FH, H_2^+ , HD^+ , and D_2^+ Molecules," J. Chem. Phys. 84, 4988 (1986).

L. Adamowicz and R.J. Bartlett, "Accurate Numerical Orbital MBPT/CC Study of the Electron Affinity of Fluorine and the Dissociation Energy of Hydrogen Fluoride," J. Chem. Phys. 84, 6837 (1986).

H. Sekino and R.J. Bartlett, "Frequency Dependent Non-linear Optical Properties of Molecules," J. Chem. Phys. 85, 976 (1986).

L. Adamowicz and R.J. Bartlett, "Coupled-Cluster Calculations of Electron Affinities of LiF," Chem. Phys. Lett. 129, 159 (1986).

H. Sekino and R.J. Bartlett, "Nuclear Spin-Spin Coupling Constants Evaluated Using Many-Body Methods," J. Chem. Phys. 85, 3945 (1986).

L. Adamowicz and R.J. Bartlett, "Direct Coupled Cluster Calculations of Excited States," Int. J. Quantum Chem. Symp. 19, 217 (1986).

E.A. Salter, L. Adamowicz, and R.J. Bartlett, "Comment on MBPT/CC Nickel Calculations," Chem. Phys. Lett. 130, 152 (1986).

S.J. Cole and R.J. Bartlett, "Comparison of MBPT and Coupled-Cluster Methods with Full CI. II. Polarized Basis Sets," J. Chem. Phys. 86, 873 (1987).

J. Noga, R.J. Bartlett and M. Urban, "Towards and Full CCSDT Model for Electron Correlation II. CCSDT-n Models," Chem. Phys. Lett. 134, 126 (1987).

L. Adamowicz and R.J. Bartlett, "MBPT and Coupled-Cluster Calculation on the Neon Atom with Numerical Orbitals," Int. J. Quantum Chem. 31, 173 (1987).

E.A. Salter, H. Sekino and R.J. Bartlett, "Orbital Relaxation and Property Evaluation by Coupled-Cluster Methods," *J. Chem. Phys.* 87, 502 (1987).

J. Noga and R.J. Bartlett, "The Full CCSDT Model for Molecular Electronic Structure," *J. Chem. Phys.* 86, 7041 (1987).

M. Rittby and R.J. Bartlett, "An Open-Shell Restricted Coupled-Cluster Method: Application to Ionization Potentials in N_2 ," *J. Phys. Chem.*, in press.

L. Adamowicz and R.J. Bartlett, "Excited State Electron Affinities of NaF, LiCl and NaCl," *J. Chem. Phys.* 88, 313 (1988).

R.J. Bartlett, S.J. Cole, G. D. Purvis, W.C. Ermler, H.C. Hsieh and I. Shavitt, "The Quartic Force Field of H_2O Determined by Many-Body Methods II. Effects of Triple Excitations," *J. Chem. Phys.* 87, 6579 (1987).

D.H. Magers, E.A. Salter, R.J. Bartlett, C. Salter, B.A. Hess and L.J. Schaad, "Do Stable Isomers of N_3H_3 Exist?," *J. Am. Chem. Soc.*, in press.

T. Pluta, A.J. Sadlej and R.J. Bartlett, "Polarizability of OH^- ," *Chem. Phys. Lett.* 143, 91 (1988).

G.D. Purvis III, H. Sekino and R.J. Bartlett, "Multiplicity of Many-Body Wavefunctions Using Unrestricted Hartree-Fock Reference Functions," *Coll. of Czechoslovak Chem. Comm.*, in press.

M. Urban and R.J. Bartlett, "MBPT and Coupled-Cluster Investigation of Isomerization Reactions: $HCN \leftrightarrow HNC$, $BH_3CH^- \leftrightarrow BH_3NC^-$ and $HCNBH_3 \leftrightarrow HNCBH_3$," *J. Am. Chem. Soc.*, submitted.

G.W. Trucks, J. Noga and R.J. Bartlett, "Convergence of Coupled Cluster Singles, Doubles and Triples Method," *Chem. Phys. Lett.*, in press.

INVITED PRESENTATIONS (1986 - present)

| | | |
|-------|------|--|
| Sept. | 1988 | ACS Conference on Analytical Derivatives and Molecular Properties, Los Angeles, CA. |
| Aug. | 1988 | Sixth International Congress on Quantum Chemistry, Jerusalem, Israel. |
| June | 1988 | Workshop on Quantum Chemistry, Basic Aspects, Actual Trends, Girona, Spain. |
| Feb. | 1988 | Workshop and Symposium on Aspects of Many-Body Effects in Molecules and Extended Systems, Calcutta, India. |
| Sept. | 1987 | National ACS Meeting, Symposium on Bound and Temporary Anions in Chemical Systems, New Orleans, LA. |
| July | 1987 | American Conference on Theoretical Chemistry, Gull Lake, MN. |
| June | 1987 | The Ninth Annual West Coast Theoretical Chemistry Conference, Berkeley, CA. |
| May | 1987 | Fifth School of Advanced Methods of Quantum Chemistry, "Frontiers of Atomic and Molecular Structure Theory," Bachotek, Poland. |
| April | 1987 | National ACS Meeting, Symposium on Applications of New Methods for Correlated <u>Ab Initio</u> Studies of Large Molecules, Denver, CO. |

| | | |
|-------|------|---|
| April | 1987 | National APS Meeting, Division of Atomic Molecular and Optical Physics, Symposium on Many-Body Physics, Crystal City, VA. |
| March | 1987 | Parr/Eliel Symposium, Chapel Hill, NC. |
| June | 1986 | Canadian Symposium on Theoretical Chemistry, Toronto, Ontario, Canada |
| April | 1986 | Workshop on Interface between Electronic Structure and Dynamics, Snowbird, Utah. |

III. Non-refereed Papers - None

IV. Honors

Rodney J. Bartlett has been promoted from Professor to Graduate Research Professor of Chemistry and Physics. The latter rank, which is the highest offered by the University of Florida, is held by only 2% of the faculty.

Three of Dr. Bartlett's papers (published 1978-1981) and supported by AFOSR have recently been designated as Science Citations Classics. Classics are determined by frequency of citation by other scientists and must be among the most cited papers in their respective journals. His paper in Physica Scripta 21, 255 (1980), "Molecular Applications of Coupled-Cluster and Many-Body Perturbation Methods," in the Proceedings of Nobel Syposium Issue, is the third most cited paper in the history of that journal, being cited over 160 times. His paper from the International Journal of Quantum Chemistry 14, 561 (1978), "Many-Body Perturbation Theory, Coupled Pair Many Electron Theory, and the Importance of Quadruple Excitations for the Correlation Problem," has been cited over 200 times, and is the eighth most cited paper in that journal's history. His review in Annual reviews of Physical Chemistry 32, 359 (1981), "Studies of Electron Correlation in Molecules with Many-Body Perturbation Theory and Coupled Cluster Methods," has also been cited over 200 times, and is the twelfth most cited paper in that review series.

V. Patent Requests - None

VI. Patents Granted - None

VII. Students Supported by Grant

- D. Bernholdt
- D. Magers
- S. Zarrabian
- E.A. Salter
- G. Trucks
- T. Pluta

| | |
|---------------------|-------------------------|
| Accession For | |
| NTIS GRA&I | |
| DTIC TAB | |
| Unannounced | |
| Justification | |
| By _____ | |
| Distribution/ _____ | |
| Availability Codes | |
| Dist | Avail and/or Special |

A-1



VIII. Postdoctoral Associates Supported by Grant

S. Pal
M. Rittby
G. Fitzgerald
L. Adamowicz
C. Sosa
J. Watts
R.E. Brown (visiting research associate)
S. Kucharski (visiting research associate)

IX. Students Under AFOSR Support Graduated

S. Zarrabian - Convergence to the Solution of the Eigenvalue Problem by Perturbative Methods (December, 1987)

E.A. Salter - Analytical One-Electron Response Properties, Molecular Gradients and Force Constants in Many-Body Methods (May, 1988)

END

DATED

FILM

8 = 88
DTIC